Signatures of non-Markovianity in classical single-time probability distributions

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Abstract. We show that the Kolmogorov distance allows to quantify memory effects in classical stochastic processes by studying the evolution of the single-time probability distribution. We further investigate the relation between the Kolmogorov distance and other sufficient but not necessary signatures of non-Markovianity within the classical setting.

1. Introduction

In the theory of classical stochastic processes the definition of Markov process relies on a requirement involving the entire hierarchy of conditional probability distributions [1]. A non-Markov process is then defined to be a stochastic process whose conditional probabilities do not comply with this requirement. In particular, the transition probabilities of a Markov process obey the well-known Chapman-Kolmogorov equation, which in the homogeneous case can be read as a semigroup composition law for a family of transition operators defined in terms of the transition probabilities of the process [1]. A Markov process can be considered as a process that lacks memory, whereas non-Markov processes describe phenomena in which memory effects are relevant.

Different approaches to the notion of stochastic process in quantum mechanics have been developed, based on C^*-algebras [2, 3, 4] or on the stochastic Schrödinger equation [5, 6, 7], just to mention some relevant examples, but there is not a well-established general theory of quantum stochastic processes. The crucial difference between the quantum and the classical setting traces back to the peculiar role played by measurement in the quantum case. In order to make statements about the values of observables of a quantum system at different times one has to specify measurement procedures, which modify the subsequent evolution [8]. The generic dynamics of a quantum system, also taking the interaction with its environment into account, i.e. the dynamics of an open quantum system [9], is usually formulated by means of a one-parameter family of completely positive dynamical maps, which fixes the evolution of the statistical operator representing the open system's state. Within this framework, where a straightforward translation of the classical definition does not apply, the non-Markovianity of a quantum dynamics has recently been defined and quantified in terms of specific properties of the dynamical maps [10, 11, 12, 13]. In analogy with the transition operators of classical Markov processes, one can identify quantum

Markovianity with a proper composition law of the dynamical maps [12], which reduces to the semigroup law in the time-homogeneous case. In a different and non-equivalent way [14, 15], one can identify quantum Markovianity with the contractivity of the trace distance between states of the open quantum system during the dynamics [11]. The trace distance quantifies the distinguishability of quantum states [16], so that its variations in the course of time can be read in terms of an information flow between the open system and its environment [11, 14, 13]. An increase of the trace distance indicates that the information is flowing from the environment to the open system, so that the influence the open system has had on the environment affects the open system back again. The trace distance allows to formulate the physical idea of memory effects as typical of non-Markovian dynamics in a mathematically definite way.

The precise relation between the definition of Markov stochastic process and the different notions of quantum Markovianity has been investigated in [17, 18]. More specifically, one can introduce also at the classical level a family of dynamical maps which describes the evolution of the single-time probability distribution of a stochastic process. The properties used to define the Markovianity of quantum dynamics naturally induce signatures of non-Markovianity for the classical stochastic processes. The evolution of the single-time probability distribution does not allow to assess the Markovianity of a stochastic process. However, the violation of either of the above-mentioned properties provides a sufficient condition for the stochastic process to be non-Markovian [17, 18]. In this paper, we deepen the analysis of the signatures of non-Markovianity and our entire discussion will be kept within the classical setting. We first focus on the signature of non-Markovianity based on the evolution of the distinguishability between single-time probability distributions, which is quantified through the Kolmogorov distance, i.e., the classical counterpart of the trace distance. In particular, we show that the increase in time of the Kolmogorov distance provides a quantitative description of the memory effects present in the evolution of single-time probability distributions. We take into account two-site semi-Markov processes [1], which allow for a complete characterization in terms of a waiting time distribution. By means of the Kolmogorov distance, we study how the different features of the waiting time distribution influence the memory effects in the subsequent evolution and then the possibility to detect the non-Markovianity of the process at the level of single-time probability distributions. Furthermore, we investigate the relation between the Kolmogorov distance and the differential equation satisfied by the single-time probability distribution. The latter is strictly related to the composition law of the classical dynamical maps and it provides a further signature of non-Markovianity, which is shown not to be equivalent to the increase of the Kolmogorov distance.

2. Memory effects in semi-Markov processes

For the sake of simplicity, let us consider a stochastic process taking values in a finite set. The single-time probability distribution at time t is then a probability vector $\boldsymbol{p}(t)$, so that its elements denoted as $p_k(t)$ $k = 1, \dots N$, satisfy $p_k(t) \geq 0$ and $\sum_k p_k(t) = 1$. As in the quantum setting [9], one can describe the time evolution of $\boldsymbol{p}(t)$ by means of a one-parameter family of dynamical maps $\{\Lambda(t,0)\}_{t\geq 0}$

$$\boldsymbol{p}(t) = \Lambda(t,0)\,\boldsymbol{p}(0)\,, \tag{1}$$

with $t_0 = 0$ fixed initial time. It is easy to see that a matrix Λ associates probability vectors to probability vectors if and only if its entries $(\Lambda)_{jk}$ satisfy the conditions:

$$(\Lambda)_{jk} \geq 0 \qquad \sum_{j=1}^{N} (\Lambda)_{jk} = 1, \tag{2}$$

$\forall j, k = 1, \ldots, N$. A matrix which fulfills equation (2) is usually called stochastic matrix. We will thus require that every dynamical map $\Lambda(t, 0)$ is a stochastic matrix.

As long as only the single-time probability distribution is taken into account, one cannot in general determine whether the stochastic process is Markovian or not. Nevertheless, one can introduce signatures of non-Markovianity at the level of the evolution of single-time probability distributions. These can be understood as sufficient but not necessary conditions for the process to be non-Markovian. The Kolmogorov distance $D_K\left(\boldsymbol{p}^1, \boldsymbol{p}^2\right)$ between two probability distributions $\boldsymbol{p}^1$ and $\boldsymbol{p}^2$ on a common finite set $\mathcal{X}$ is defined as

$$D_K\left(\boldsymbol{p}^1, \boldsymbol{p}^2\right) = \frac{1}{2} \sum_{k \in \mathcal{X}} \left|p_k^1 - p_k^2\right|. \tag{3}$$

Now, consider the time evolution of the Kolmogorov distance $D_K\left(\boldsymbol{p}^1(t), \boldsymbol{p}^2(t)\right)$ between probability vectors evolved from different initial conditions through the stochastic matrix in (1). The Chapman-Kolmogorov equation implies [17] $D_K\left(\boldsymbol{p}^1(t), \boldsymbol{p}^2(t)\right) < D_K\left(\boldsymbol{p}^1(s), \boldsymbol{p}^2(s)\right)$, $\forall t \geq s$, so that any revival in the evolution of the Kolmogorov distance is a signature of the non-Markovianity of the process. By adapting the interpretation introduced for the dynamics of open quantum systems [11, 13], any increase of the Kolmogorov distance can be read as a memory effect in the evolution of the single-time probability distribution. The information about the initial condition that is contained in the initial value of the Kolmogorov distance can be partially lost and then recovered, implying an increase of the distinguishability between the probability distributions evolved from the two different initial conditions. We can quantify the memory effects in the overall dynamics fixed by the stochastic matrices $\Lambda(t, 0)$ by integrating the rate of change of the Kolmogorov distance $\sigma(t, \boldsymbol{p}^{1,2}(0)) = (\mathrm{d}/\mathrm{d}t) D_K\left(\boldsymbol{p}^1(t), \boldsymbol{p}^2(t)\right)$ over the time-intervals where the information about the initial condition is recovered. Namely, we define (compare with [11])

$$\mathcal{N}_C(\Lambda) = \max_{\boldsymbol{p}^{1,2}(0)} \int_{\sigma > 0} \mathrm{d}t \, \sigma(t, \boldsymbol{p}^{1,2}(0)), \tag{4}$$

where the maximum among the couples of initial probability vectors is taken. $\mathcal{N}_C(\Lambda)$ points out the relevance of the signature of non-Markovianity in the evolution of single-time probability distributions given by the increase of the Kolmogorov distance.

As a specific example, let us consider the semi-Markov processes [1], which are a class of stochastic processes allowing for a compact characterization. The semi-Markov processes combine features of Markov chains and renewal processes [19]: they describe a system moving among different sites in a way such that the random times separating the different transitions as well as the transition probabilities between the different sites only depend on departure and arrival sites. A semi-Markov process is completely determined by the semi-Markov matrix $Q(t)$, whose entries $(Q)_{jk}(t)$ are the probability densities to make the jump $k \to j$ in a time t. For the sake of simplicity, we will take into account a system moving between two different sites and a semi-Markov matrix $Q(t) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} f(t)$. This means that once in a site the system

jumps with certainty to the other, with a random time before each new jump given by the site-independent waiting time distribution $f(t)$. The semi-Markov process will be Markovian according to the precise definition of the classical stochastic processes if and only if the waiting time distribution is the exponential one [20]

$$g(t) \equiv \lambda e^{-\lambda t}. \tag{5}$$

For a generic waiting time distribution, the dynamical maps $\Lambda(t,0)$, which can be obtained through an integrodifferential equation fixed by the semi-Markov matrix [17], are

$$\Lambda(t,0) = \frac{1}{2}\begin{pmatrix} 1+q(t) & 1-q(t) \\ 1-q(t) & 1+q(t) \end{pmatrix}. \tag{6}$$

Here, $q(t) = \sum_{n=0}^{\infty} p(2n,t) - \sum_{n=0}^{\infty} p(2n+1,t)$ expresses the difference between the probability to have an even or an odd number of jumps up to time t. This quantity is related to the waiting time distribution via the corresponding Laplace transforms

$$\hat{q}(u) = \frac{1}{u}\frac{1-\hat{f}(u)}{1+\hat{f}(u)}, \tag{7}$$

where $\hat{v}(u) = \int_0^\infty \mathrm{d}t\, v(t)\, e^{-ut}$ is the Laplace transform of the function $v(t)$. The dynamical map $\Lambda(t,0)$ associates the initial probability vector to the probability vector at time t and then determines the expression of the Kolmogorov distance. In particular, for $\Lambda(t,0)$ as in (6) one has

$$D_K\left(\boldsymbol{p}^1(t), \boldsymbol{p}^2(t)\right) = |q(t)| D_K\left(\boldsymbol{p}^1(0), \boldsymbol{p}^2(0)\right). \tag{8}$$

Thus, the memory effects in the evolution of the single-time probability distribution are quantified by, see (4),

$$\mathcal{N}_C(\Lambda) = \int_{\Omega_+} \mathrm{d}t \frac{\mathrm{d}}{\mathrm{d}t}|q(t)| = \sum_i \left(|q(b_i)| - |q(a_i)|\right), \tag{9}$$

where $\Omega_+ = \bigcup_i (a_i, b_i)$ corresponds to the time intervals in which $|q(t)|$ increases. The maximum growth of the Kolmogorov distance in the course of time is obtained for the two initial probability vectors $(1,0)^\top$ and $(0,1)^\top$.

By studying the quantity $\mathcal{N}_C(\Lambda)$ in (9) for different choices of the waiting time distribution $f(t)$, we can describe how different semi-Markov processes are characterized by a different amount of memory effects in the evolution of $\boldsymbol{p}(t)$. An interesting class of waiting time distributions is given by the so-called special Erlang distributions of order n. The latter consist in the convolution of n equal exponential waiting time distributions of parameter λ, see (5):

$$f(t) = \underbrace{(g * \ldots g)}_{n}(t). \tag{10}$$

A special Erlang distribution of order n describes a random variable given by the sum of n independent and identically distributed exponential random variables. This waiting time distribution can be related to a system that jumps from one site to another in various unobserved stages. Each stage is exponentially distributed in time, but one observes only when n stages have occurred. In this situation, the non-Markovianity expressed by the non-exponential waiting time distribution is due to the lack of information about all the intermediate stages [20]. Indeed, one expects that the higher is the number of unobserved stages the stronger is the deviation from the Markovian situation. Now, $\mathcal{N}_C(\Lambda)$ allows to formulate this statement in

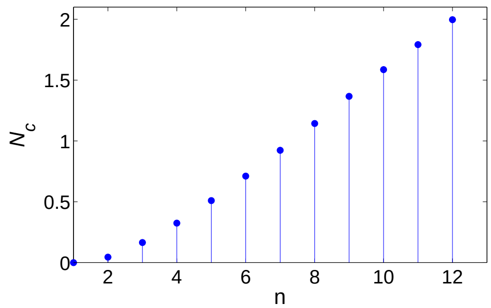

Figure 1. Size of memory effects in the evolution of $\boldsymbol{p}(t)$ for a two-site semi-Markov process versus the number n of the exponential distributions in the special Erlang waiting time distribution (10) that fixes the process. The memory effects are quantified by means of $\mathcal{N}_C(\Lambda)$ defined in (9), where $q(t)$ is obtained through equation (7). For $n = 2$, $\mathcal{N}_C(\Lambda) = 0.045$ (compare with figure 2).

a precise way since it quantifies the memory effects in the evolution of $\boldsymbol{p}(t)$, which represent a signature of non-Markovianity. In figure 1, we plot $\mathcal{N}_C(\Lambda)$ for a semi-Markov process that describes a system moving between two different sites with a waiting time distribution as in (10). For $f(t) = \lambda e^{-\lambda t}$ the Kolmogorov distance is monotonically decreasing [17], so that $\mathcal{N}_C(\Lambda) = 0$. Then, $\mathcal{N}_C(\Lambda)$ increases with the number of exponential distributions in (10) and, quite remarkably, it grows to a good approximation in a linear way for $n > 3$. The memory introduced by the lack of information about intermediate stages growths linearly with the number of unobserved stages. In addition, let us note that $\mathcal{N}_C(\Lambda)$ does not depend on the parameter λ in (10). By the properties of the Laplace transform or by dimensional analysis, one can easily find that $q(t)$ is a function of λt. Maxima and minima of $q(t)$ do not depend on λ and thus neither does $\mathcal{N}_C(\Lambda)$, see the right hand side of (9). Only the functional expression of the waiting time distribution matters.

As a further example, we consider the convolution of two non-exponential waiting time distributions. Coming back to the picture of a system jumping between two sites with unobserved stages, we study how the memory in the evolution of $\boldsymbol{p}(t)$ is influenced by the specific waiting time distribution that characterizes the intermediate stages. Let the waiting time distribution $f(t)$ be the convolution of two equal mixtures of exponential distributions with rates, respectively, λ_1 and λ_2: given $h(t) \equiv \mu\lambda_1 e^{-\lambda_1 t} + (1-\mu)\lambda_2 e^{-\lambda_2 t}$, we set

$$f(t) = (h * h)(t). \tag{11}$$

A mixture $\sum_k \mu_k f_k(t)$ describes a system that moves between different sites following with probability μ_k the distribution $f_k(t)$. Thus, $f(t)$ as in (11) means that both the unobserved stages are exponentially distributed in time with a rate that is given by λ_1, with probability μ, or by λ_2, with probability $1-\mu$. In figure 2, we plot the evolution of $|q(t)|$, see (7), for $f(t)$ as in (11). Recall that $|q(t)|$ is the Kolmogorov distance for the two initial probability vectors that maximize $\mathcal{N}_C(\Lambda)$, see (9). Moreover, if the waiting time distribution is simply the mixture of two exponential distributions, then the Kolmogorov distance is monotonically decreasing [17], so that $\mathcal{N}_C(\Lambda) = 0$. We can see in figure 2 that this is still the case for the convolution of two mixtures with balanced exponential distributions, i.e., $\mu = 1/2$. Even more, only a strong imbalance between

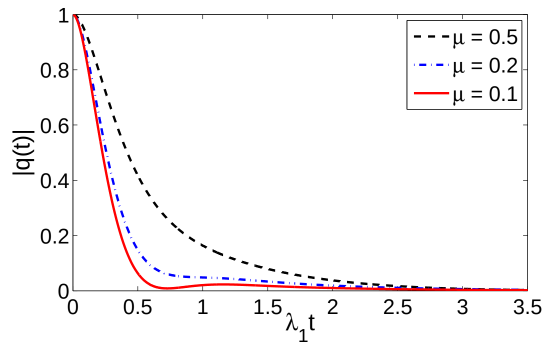

Figure 2. Plot of $|q(t)|$ versus time for a waiting time distribution given by the convolution of two equal mixtures of exponential distributions, see (11), for different values of the mixing parameter μ; in addition, $\lambda_2/\lambda_1 = 5$. $\mathcal{N}_C(\Lambda)$ in (9) is equal to 0 for $\mu = 0.5$ and $\mu = 0.2$, while $\mathcal{N}_C(\Lambda) = 0.022$ for μ=0.1.

the weights of the two exponential distributions provides an increase of the Kolmogorov distance, witnessing the presence of memory effects. In any case, this signature of non-Markovianity is smaller than for the convolution of two equal exponential distributions, i.e., for $f(t)$ as in (10) with $n = 2$, which is recovered from (11) for $\mu = 0$ or $\mu = 1$. If the rate of the exponential distributions of the unobserved stages is not known with certainty, the memory due to the lack of information about the occurrence of the stages is reduced. In particular, if the available exponential distributions are equally probable, there will be no memory effects at all.

3. Kolmogorov distance and time-local equation

In this section, we study the relation between the Kolmogorov distance and the differential equation satisfied by $\boldsymbol{p}(t)$, which provides further signatures of non-Markovianity. From the knowledge of the dynamical maps $\Lambda(t, 0)$, one can directly obtain a time-local equation in the form

$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{p}(t) = L(t)\boldsymbol{p}(t), \tag{12}$$

by means of the relation [21, 22]

$$L(t) = \frac{\mathrm{d}\Lambda(t,0)}{\mathrm{d}t}\Lambda^{-1}(t,0). \tag{13}$$

In particular, consider the case such that $L(t)$ satisfies the so-called Kolmogorov conditions for any $t \geq 0$, i.e., $(L(t))_{jk} \geq 0$ for $j \neq k$, $(L(t))_{jj} \leq 0$ and $\sum_k (L(t))_{jk} = 0$ for any j. Equation (12) is then equivalent to the system of equations

$$\frac{\mathrm{d}}{\mathrm{d}t}p_j(t) = \sum_k (W_{jk}(t)p_k(t) - W_{kj}(t)p_j(t)) \tag{14}$$

with $W_{jk}(t) \geq 0$ linked to $(L(t))_{jk}$ through $(L(t))_{jk} = W_{jk}(t) - \sum_l W_{lk}(t)\delta_{jk}$. One can show [23] that $L(t)$ satisfies the Kolmogorov conditions for any $t \geq 0$ if and only if the corresponding family of dynamical maps $\{\Lambda(t, 0)\}_{t\geq 0}$ satisfies

$$\Lambda(t, 0) = \Lambda(t, s)\Lambda(s, 0) \tag{15}$$

for any $t \geq s \geq 0$, with $\Lambda(t,s)$ itself being a stochastic matrix. The composition law (15), named P-divisibility in [17], represents the classical counterpart of the composition law exploited in [12] to define the notion of quantum Markovianity [17, 18]. The violation of P-divisibility provides a further signature of the non-Markovianity of classical stochastic processes at the level of single-time probability distributions. Note that this signature of non-Markovianity can be directly read from the time-local equation (14) since P-divisibility is violated if and only if $W_{jk}(t) < 0$ for some j,k and $t \geq 0$. As emphasized [9, 24] for the quantum dynamics of statistical operators, also the evolution of the single-time probability distribution of a classical stochastic process can be described through a time-local equation even if the process is non-Markovian. In particular, negative coefficients in the equation will account for memory effects in the evolution of $\boldsymbol{p}(t)$ [25].

For the two-site semi-Markov processes described in the previous section, with $\Lambda(t,0)$ as in (6), one has

$$L(t) = \begin{pmatrix} -\gamma(t) & \gamma(t) \\ \gamma(t) & -\gamma(t) \end{pmatrix}, \tag{16}$$

with

$$\gamma(t) = -\frac{\mathrm{d}q(t)/\mathrm{d}t}{2q(t)}. \tag{17}$$

Thus, the elements $p_j(t)$, $j = 1, 2$, satisfy the following system of differential equations:

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}p_1(t) &= \gamma(t)\left(p_2(t) - p_1(t)\right) \\ \frac{\mathrm{d}}{\mathrm{d}t}p_2(t) &= \gamma(t)\left(p_1(t) - p_2(t)\right). \end{aligned} \tag{18}$$

The rate $\gamma(t)$ in (18) is positive if and only if the corresponding Kolmogorov distance is monotonically decreasing, see (8) and (17). For these processes the increase of the Kolmogorov distance and the negativity of the coefficients in the time local equation (14), or, equivalently, the violation of P-divisibility, provide signatures of non-Markovianity that are fully equivalent. One could show that this is the case for any two-site semi-Markov process with a site-independent waiting time distribution.

Now, consider any non-Markov process whose single-time probability distribution satisfies

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}p_1(t) &= \gamma_2(t)p_2(t) - \gamma_1(t)p_1(t) \\ \frac{\mathrm{d}}{\mathrm{d}t}p_2(t) &= \gamma_1(t)p_1(t) - \gamma_2(t)p_2(t), \end{aligned} \tag{19}$$

with

$$\begin{aligned} &\gamma_2(t) < 0 \quad \text{for some } t \geq 0; \quad \gamma_1(t) \geq 0 \quad \forall\, t \geq 0 \\ &\gamma_1(t) + \gamma_2(t) \geq 0 \quad \forall\, t \geq 0. \end{aligned} \tag{20}$$

If we further ask $\int_0^t \mathrm{d}\tau \gamma_2(\tau) \geq 0$ for any $t \geq 0$ the resulting dynamics is well-defined, i.e. the positivity of $\boldsymbol{p}(t)$ is conserved. By solving (19), one easily finds

$$D_K\left(\boldsymbol{p}^1(t), \boldsymbol{p}^2(t)\right) = e^{-\int_0^t \mathrm{d}\tau(\gamma_1(\tau)+\gamma_2(\tau))} D_K\left(\boldsymbol{p}^1(0), \boldsymbol{p}^2(0)\right), \tag{21}$$

which is a monotonically decreasing function because of the last condition in (20). Thus, there are processes such that the Kolmogorov distance $D_K\left(\boldsymbol{p}^1(t), \boldsymbol{p}^2(t)\right)$ does not increase in time, even if there is some negative coefficient in the time-local equation (14), see the first condition in (20), so that P-divisibility is violated: these signatures of non-Markovianity are in general not equivalent.

4. Conclusions

We have investigated signatures of non-Markovianity in the evolution of the single-time probability distribution $\boldsymbol{p}(t)$ of classical stochastic processes. We have first focused on the increase of the Kolmogorov distance between probability vectors. This allows to detect memory effects related to the initial condition in the subsequent evolution of $\boldsymbol{p}(t)$ and it naturally leads to the introduction of a quantity that measures the relevance of the memory effects, which can be seen as the classical counterpart of the measure for quantum non-Markovianity introduced in [11]. We have then discussed the relation between the increase of the Kolmogorov distance and the time-local equation satisfied by the probability vector. We have shown how for two-site semi-Markov processes with a site-independent waiting time distribution the negativity of the rates in the time-local equation is equivalent to a non-monotonic evolution of the Kolmogorov distance, further presenting examples for which this is not the case.

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